

On Tree Based Phylogenetic Networks

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Abstract.— A large class of phylogenetic networks can be obtained from trees by the addition of horizontal edges between the tree edges. These networks are called tree based networks. Reticulation-visible networks and child-sibling networks are all tree based. In this work, we present a simply necessary and sufficient condition for tree-based networks and prove that there is a universal tree based network N for each set of species such that every phylogenetic tree on the same species is a base of N . The existence of universal tree based network implies that for any given set of phylogenetic trees (resp. clusters) on the same species there exists a tree base network that display all of them.

Keywords: Phylogenetic tree, phylogenetic network, tree base, reticulation visibility,, horizontal gene transfer

Reticulation process refers to the transfer of genes between organisms in a way other than reproduction. One of the major reticulation processes is horizontal gene transfer. It has been considered as a highly significant form of genetic transfer among single-cell organisms (Doolittle, 1999; Doolittle and Baptiste, 2007; Smets and Barkay, 2006; Treangen and Rocha, 2011). Other reticulation processes include introgression, recombination and hybridization (Dagan and Martin, 2006; Fontaine et al., 2015; McBreen and Lockhart, 2006).

A set of gene trees are usually reconciled into a phylogenetic network to model reticulation processes (Doolittle and Baptiste, 2007; Huson, Rupp, and Scornavacca, 2011). A phylogenetic network is a rooted acyclic digraph in which there is a special node of out-degree 2 and in-degree 0 (called the root) such that all the edges are directed away from it and the set of in-degree 0 nodes correspond one-to-one the collection of present-day taxa under study. A network is binary if every node other than the root and leaves is of degree three. Clearly, a phylogenetic tree is a binary phylogenetic network without reticulation nodes.

Horizontal gene transfers are naturally modeled and visualized by using a tree-based phylogenetic network, where the underlying base tree represents the evolution of the species from which genes are sampled and branches are added between tree branches to represent horizontal gene transfers (Smets and Barkay, 2006; Nakhleh, 2013). Surprisingly, phylogenetic networks that are used for modeling other reticulation processes may also have the same topological structure, obtained from a tree by the addition of branches between tree branches, even if not every binary phylogenetic network shares this property (van Iersel, 2013). Recently, Francis and Steel (2015) initiated the study of tree-based networks. In their paper, sufficient conditions for tree-based networks are presented. They further showed that this class of networks include reticulation visible networks and tree-sibling networks.

In the present work, we answer two problems posed by Francis and Steel (2015). Precisely, we present a simple necessary and sufficient condition for tree-based networks. We also construct a universal network on X that has every tree on X as its base for any X of an arbitrary size.

TREE-BASED NETWORKS

Basic Definitions

A digraph D consists of a set of vertexes, $V(D)$, and a collection of directed edges, $E(D)$, that each connects an ordered pair of vertexes. We call $(u, v) \in E(D)$ an outgoing edge of u and an incoming edge of v . For each $x \in V(D)$, the number of the incoming edges of x is called its *indegree*; the number of the outgoing edges of x is called its *outdegree*; the sum of the indegree and outdegree of x is called its *degree*. The indegree, outdegree, and degree of x are written $d^i(x)$, $d^o(x)$ and $d(x)$, respectively.

A path from x to y in D is made up of two or more “successive” vertexes $x = u_1, u_2, \dots, u_k = y$, where $(u_i, u_{i+1}) \in E(D)$ for $1 \leq i \leq k - 1$ and $k \geq 2$. A cycle is a path from a node to itself. D is acyclic if it does not contain any cycle.

A binary phylogenetic network over a set X of species is an acyclic digraph with the following properties:

- There exists a unique vertex ρ such that $d^i(\rho) = 0$. It is the *root* of the network. The root is of outdegree 2.
- There are exactly $|X|$ nodes ℓ such that $d^i(\ell) = 1$ and $d^o(\ell) = 0$, corresponding one-to-one with the species. These nodes are called the *leaves* of the network.
- All the vertexes that are neither a leaf nor the root are of degree three. They are called *internal nodes*.

An internal node x in a binary phylogenetic network is called a *tree* (or *speciation*) *node* if $d^i(x) = 1$ and $d^o(x) = 2$; it is called a *reticulation node* if $d^i(x) = 2$ and $d^o(x) = 1$. Since the root is the only vertex having indegree 0 in a phylogenetic network, there is a path from the root to every other vertex. For two vertexes x and y , if there is a path from y to x , y is said to be an *ancestor* of x and x is said to be a *descendant* of y .

A binary phylogenetic networks is shown in Figure 1, where we draw an open branch entering the root, representing the least common ancestor of all the species. In rest of the paper, for a binary phylogenetic network N , we shall use the following notation:

- ρ_N : The root of N ;
- $\mathcal{V}(N)$: The set of nodes in N ;
- $\mathcal{T}(N)$: The set of tree nodes in N ;
- $\mathcal{R}(N)$: The set of reticulation nodes in N ;
- $\mathcal{E}(N)$: The set of (directed) edges in N ;
- $\mathcal{L}(N)$: The set of labelled leaves in N ;
- $c(u)$: The unique child of u if $u \in \mathcal{R}(N)$, or the set of the children of u if $u \in \mathcal{T}(N)$;

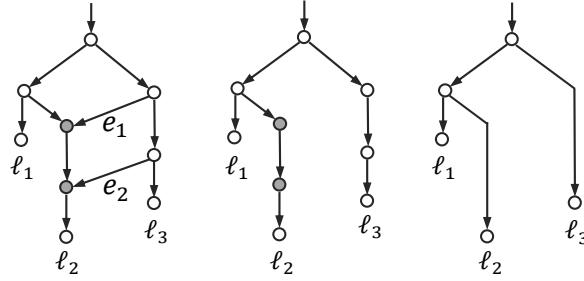


Figure 1: A tree-based phylogenetic network (left) and a tree base of it (right). The subdivision of the base tree (middle) is a subtree of the network that can be obtained by the removal of the edges e_1 and e_2 . Reticulation nodes in the network are represented by shaded circles,

- $p(u)$: The unique parent of u if $u \in \mathcal{T}(N)$, or the set of the parents of u if $u \in \mathcal{R}(N)$;

Tree-based networks

Let N be a network over a set of species, X . For a subset $E \subseteq \mathcal{E}(N)$, $N - E$ denotes the subnetwork of N obtained after the removal of the edges in E . If E contains exactly an incoming edge for each reticulation vertex, then every non-root node in $N - E$ is of indegree 1 and hence is a tree. However, it may contain new leaves. N is *tree-based* if there exists $E \subseteq \mathcal{E}(N)$ such that $N - E$ is a subtree having the same leaves as N .

The network in Figure 1 is tree-based. It has two reticulation vertexes. The edge e_1 enters the top reticulation vertex, whereas e_2 is an edge entering the other at the bottom. The removal of these two edges results in a subtree with the same leaves as the network. On the other hand, the network in Figure 2A is not tree-based. The reason is that no matter which of the incoming edges (r_1, r_4) and (r_2, r_4) is removed for r_4 , the tail of the removed edge becomes a new leaf in the resulting subtree.

Tree-based networks compose of a large class of interesting networks. A vertex in a phylogenetic network is called *visible* (or *stable*) if there exists a leaf such that every path from the network root to the leaf passes through the vertex. A network is *reticulation visible* if every reticulation vertex is visible. Reticulation visible networks are tree-based (Francis and Steel, 2015; Gambette *et al.*, 2015).

A phylogenetic network is *tree sibling* if every reticulation vertex has a tree vertex sibling. Tree sibling networks are also tree based (Francis and Steel, 2015).

MAIN RESULTS

A necessary and sufficient condition for tree-based networks

In a binary phylogenetic network, a reticulation vertex is said to be of:

- *type-0* if its parents are both a reticulation vertex;
- *type-1* if a parent is a reticulation vertex and the other is a tree vertex;
- *type-2* if its parents are both a tree vertex.

In the network drawn in Fig 2A., the vertexes r_1, r_2 and r_3 are of type-2, r_5 is of type-1, and r_4 is of type-0. A tree-based network must not contain any type-0 reticulation vertexes (Francis and Steel, 2015).

Let N be a binary phylogenetic network without type-2 vertexes. Setting $\mathcal{R}(N) = \{r_1, r_2, \dots, r_s\}$, we define an undirected bipartite graph $B(N) = (X \cup Y, E)$ as follows:

$$\begin{aligned} X &= \{x_1, x_2, \dots, x_s \mid x_i \text{ represents } r_i \text{ for each } i\}, \\ Y &= \{y_1, y_2, \dots, y_t \mid y_i \text{ represents a parent in } \mathcal{T}(N) \text{ of a vertex in } \mathcal{R}(N) \}, \end{aligned}$$

and

$$E = \{(y_j, x_i) \mid \text{the vertex represented by } y_j \text{ is a parent of the vertex by } x_i \text{ in } N.\}.$$

Remark that $B(N)$ is essentially a bipartite subgraph of N . For example, Figure 2B shows the bipartite network defined for the network in Figure 2A, in which x_4 is not connected with any other vertex, as the parents of r_4 are both not a tree vertex.

Using the technique of Gambette et al. (2015), we are able to present a simple necessary and sufficient condition for binary tree-based phylogenetic networks.

Lemma 1 *Let N be a network without type-0 reticulation vertexes. Then N is tree-based if and only if for every two type-1 reticulation vertexes, their correspondences are not connected in B_N .*

Proof. First, we have the following two facts:

(i) Let $e = (x, y) \in \mathcal{E}(N)$. If x is a reticulation vertex, then x has out-degree 0 and hence becomes a leaf in $N - \{e\}$.

(ii) Let $e_1 = (x_1, y_1) \in \mathcal{E}(N)$ and $e_2 = (x_2, y_2) \in \mathcal{E}(N)$ such that $x_i \in \mathcal{T}(N)$ and $y_i \in \mathcal{R}(N)$ for $i = 1, 2$. If $x_1 = x_2$, then x_1 becomes a leaf in $N - \{e_1, e_2\}$. If $y_1 = y_2$, then y_1 has in-degree 0 in $N - \{e_1, e_2\}$.

Each edge (t, r) in N corresponds an edge in $B(N)$, where $t \in \mathcal{T}(N)$ and $r \in \mathcal{R}(N)$. For a subset $E \subseteq \mathcal{E}(N) \cap (\mathcal{T}(N) \times \mathcal{R}(N))$, we set $E_{B(N)}$ to be the subset of edges in $B(N)$ that correspond one-to-one to the edges in E . The two facts stated above imply that $N - E$

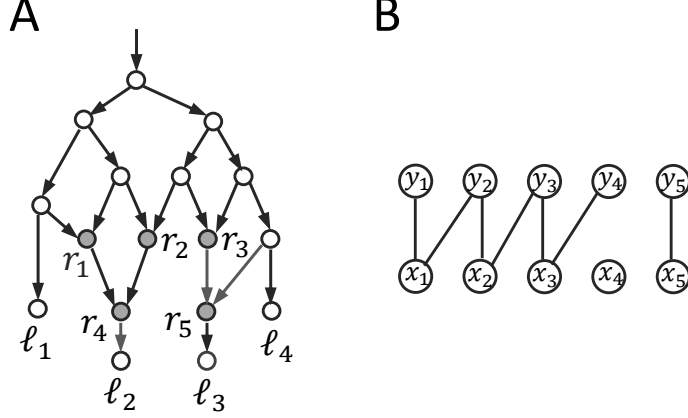


Figure 2: (A) A binary phylogenetic network N , in which reticulation vertexes are represented by shaded circles. (B) The bipartite graph $B(N)$ defined for N .

is a tree network with the same leaves as N if and only if E is a matching covering every reticulation vertex in N and hence if and only if $E_{B(N)}$ is a complete matching from X to Y in $B(N)$.

Since $B(N)$ is bipartite, by Hall's theorem, there is a complete matching from X to Y if and only if $|X'| \leq |N(X')|$ for any $X' \subseteq X$, where $N(X')$ is the set of vertexes that are adjacent with some vertexes in X' , and so if and only if there is a complete matching from $C \cap X$ to $C \cap Y$ for every connected component C in $B(N)$.

A vertex x_i in $B(N)$ is of degree 1 if it corresponds a type-1 reticulation vertex; it is of degree 2 if it corresponds a type-2 reticulation vertex. Each vertex y in $B(N)$ has also degree 1 or degree 2, as the tree vertex represented y has one or two reticulation children. Therefore, every connected component is either a cycle or a path in $B(N)$. Let C be a connected component in $B(N)$. If C is a cycle, C has a perfect matching from $C \cap X$ to $C \cap Y$. If C is a path, it contains exactly two degree-1 vertexes w' and w'' . There is a complete matching from $C \cap X$ to $C \cap Y$ if and only if either w' or w'' is not in X .

Since the degree-1 vertexes in X correspond one-to-one to the type-1 reticulation vertexes, we conclude that N is tree-based if and only if the correspondences of every two type-1 reticulation vertexes are not connected in $B(N)$. \square

Let $u, v \in \mathcal{R}(N)$. We say that they are connected by a *zigzag* path if there is a sequence of vertexes $u = x_0, x_1, \dots, x_{2k} = v$ such that the vertexes alternate between reticulation vertexes and their tree vertex parents (Figure 3).

Recalled that $B(N)$ is a disjoint union of paths and cycles. Obviously, each cycle contains only type-2 reticulation vertexes. Each type-1 reticulation vertex appears only at the ends of a path. Therefore, by Lemma 1, we have the following theorem.

Theorem 1 *Let N be a binary network. N is tree-based if and only if (i) there is no type-0 reticulation vertex in N , and (ii) no two type-1 vertexes are connected by a zigzag path.*

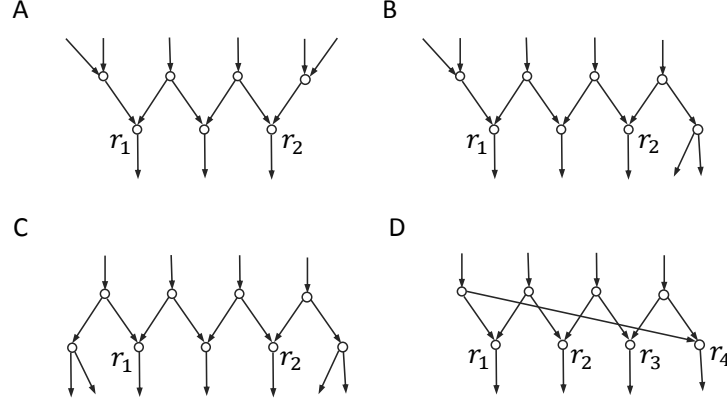


Figure 3: (A) A maximal zigzag path between two type-1 reticulation vertexes r_1 and r_2 . (B) A maximal zigzag path between a type-1 reticulation vertex r_1 and a type-2 reticulation vertex r_2 . (C) A maximal zigzag path between two type-2 reticulation vertexes r_1 and r_2 . (D) A zigzag cycle consisting of only type-2 reticulation vertexes.

Theorem 1 implies the following algorithm for determining whether a network is tree-based or not.

Input A binary network N ;

1. **If** it contains a type-0 reticulation vertex, **output** “ N is not tree-based”;
 2. **Do** until there is no unmarked type-1 reticulation vertex {
 - Select an unmarked type-1 reticulation vertex u ;
 - If** the zigzag path starting at u terminates at an unmarked type-1 reticulation vertex, **output** “ N is not tree-based”;
 - else** mark u ;
 3. **Output** “ N is tree-based”;
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Obviously, the above algorithm is correct. Since any two zigzag paths are disjoint, it takes a linear time.

UNIVERSAL TREE-BASED NETWORKS

It is known that there exists a network that displays every phylogenetic tree on the same species (see, for example, Francis and Steel, 2015). However, a tree may be displayed, but not as a base, in a phylogenetic network. Therefore, the following question is posed by Francis and Steel:

Does there exist a network U over X such that every phylogenetic tree over X is a base for U for every large set of species X ?

For $|X| = 3$, such a universal network exists (Francis and Steel, 2015). We shall present such a universal tree-based network U for every X in the rest of this section.

Let $X = \{1, 2, \dots, m\}$, $m \geq 3$. The network U on X is divided into the upper and lower parts (Figure 4A) and (Figure 4B). The upper part is denoted by U_{upper} . It is a $(2m - 3)$ -row network in which:

- the root ρ_U is the unique vertex in the row 1, written t_{01} ;
- the row $2i$ comprises $i + 1$ tree vertexes $t_{i1}, t_{i2}, \dots, t_{i(i+1)}$ for $i = 1, 2, \dots, m - 2$;
- the row $2i + 1$ comprises i reticulation vertexes $r_{i1}, r_{i2}, \dots, r_{ii}$ for $i = 1, 2, \dots, m - 2$;
- the edge set comprises (Figure 5A):

(middle diagonal edges) $(t_{ij}, r_{ij}), (t_{i(j+1)}, r_{ij}), 1 \leq j \leq i, 1 \leq i \leq m - 2,$

(side edges) $(t_{i1}, t_{(i+1)1}), (t_{i(i+1)}, t_{(i+1)(i+2)}), 0 \leq i \leq m - 3,$

(middle vertical edges) $(r_{ij}, t_{(i+1)(j+1)}), 1 \leq j \leq i, 1 \leq i \leq m - 3.$

Figure 4C shows how the rooted binary tree $(\ell_1, (((\ell_2, \ell_3), \ell_4), \ell_5))$ is displayed in U_{upper} , in which the i -th leaf counted from left corresponds to ℓ_i , $i \leq 5$.

Lemma 2 *Let $m \geq 3$ and let U_{2m-4} consist of the vertexes in the top $2m - 4$ rows and the edges between them in U_{upper} . Then, every phylogenetic tree T over $\{1, 2, \dots, m - 1\}$ is a base of U_{2m-4} , where the j -th leaf (counted from left) in T is mapped to $t_{(m-2)j}$ for each j from 1 to $m - 1$.*

The lower part U_{lower} is essentially a rearrangeable network with m inputs and m outputs. A network with m inputs and m outputs is said to be rearrangeable if for any one-to-one mapping π of the inputs to the outputs, we can construct vertex-disjoint paths in the network linking the i th input and the $\pi(i)$ th output for $1 \leq i \leq m$ (Leighton, 1992). Figure 4D shows the vertex-disjoint paths for the mapping $\pi = (45312)$ in U_{btm} , where $m = 5$ and π maps i to the i -th digit inside the parentheses.

U_{lower} is a mimic of the rearrangeable network derived from the well-known even-odd transposition sorting process in a linear array (Leighton, 1992, page 139). The topological structure of U_{lower} is slightly different for odd m and even m . We use R_i to denote the row i in U .

When m is odd, U_{lower} is divided into $2m + 1$ rows $R_{2m-2}, R_{2m-1}, \dots, R_{4m-2}$.

- For each $i = m - 1, m + 1, \dots, 2m - 2$, R_{2i} comprises $m - 1$ tree vertexes t_{ij} ($1 \leq j \leq m - 1$); R_{2i+1} comprises $m - 1$ reticulation vertexes r_{ij} ($1 \leq j \leq m - 1$).
- For each $i = m, m + 2, \dots, 2m - 3$, R_{2i} comprise $m - 1$ tree vertexes t_{ij} ($2 \leq j \leq m$); R_{2i+1} comprises $m - 1$ reticulation vertexes r_{ij} ($2 \leq j \leq m$).
- The last row R_{4m-2} comprises m leaves labelled with j ($1 \leq j \leq m$) from left to right. For sake of convenience, the j -th leaf is denoted by $t_{(2m-1)j}$.

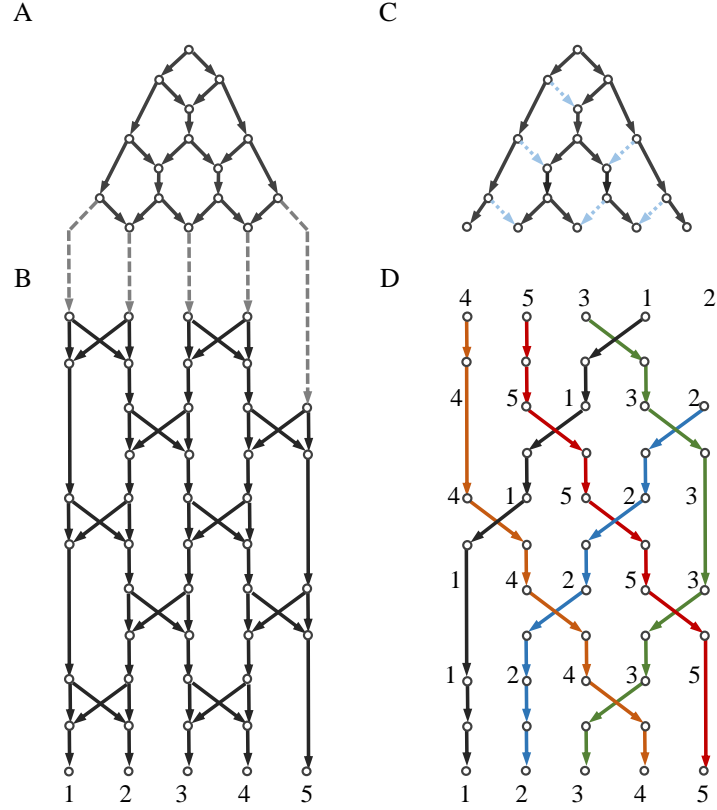


Figure 4: The universal network U with five leaves. (A) The upper part U_{upper} . (B) The lower part U_{lower} . The square dot arrows represent edges between the two parts. (C) The display of a rooted binary tree with five unlabeled leaves in U_{upper} , where the round dot arrows represent the removed edges. In this display, the i -th leaf (counted from left) in the tree is mapped to the i -th vertex in the last row. (D) The vertex-disjoint paths for the one-to-one mapping $\pi = (45312)$, where π maps i to the i -th digit inside the parentheses.

The edges in U_{lower} are formally presented in Appendix A. Briefly, for $i = m - 1 + 2j$ and $0 \leq j \leq (m - 1)/2$, the $m - 1$ vertexes in R_{2i} and R_{2i+1} are paired and connected in a butterfly, as shown in Figure 5B.

For $i = m + 2j$ and $0 \leq j \leq (m - 3)/2$ the $m - 1$ vertexes in R_{2i} and R_{2i+1} are also paired and connected in a butterfly, as shown in Figure 5C.

For $0 \leq j \leq (m - 3)/2$, the first reticulation vertex $r_{(m-1+2j)1}$ in $R_{2m+4j-1}$ is connected with the first tree vertex $t_{(m+1+2j)1}$ in $R_{2m+4j+1}$, whereas the m -th reticulation vertex $r_{(m+2j)m}$ in $R_{2m+4j+1}$ is connected with the m -th tree vertex $t_{(m+2+2j)m}$ in $R_{2m+4j+4}$.

Finally, there are also m edges between the vertexes at the bottom of U_{upper} and the corresponding vertexes on the top in U_{lower} , which are represented by the square dot arrows drawn between Figure 4A and 4B.

When m is even, the structure of U_{lower} is presented in Appendix A.

Lemma 3 *Let π be any one-to-one mapping on $\{1, 2, \dots, m\}$.*

(i) *When m is odd, there are m vertex-disjoint paths connecting $t_{(m-1)j}$ and $t_{(2m-1)\pi(j)}$ ($1 \leq j \leq m - 1$) and t_{mm} and $t_{(2m-1)\pi(m)}$ in U_{lower} .*

(ii) *When m is even, there are m vertex-disjoint paths connecting $t_{(m-1)j}$ and $t_{(2m-1)\pi(j)}$ ($1 \leq j \leq m$) in U_{lower} .*

Additionally, every vertex in U_{lower} appears in one of the m paths mentioned in (i) and (ii).

Theorem 2 *Every phylogenetic tree over X is a base for U .*

Proof. Essentially, we shall prove that for each tree T , its topological structure can be displayed in U_{upper} and the leaves are then rearranged in U_{lower} according to the order they appear in T . We just prove the theorem for odd m . (The case m is even is similar.)

Consider a phylogenetic tree T over $X = \{1, 2, \dots, m\}$. Assume that its leaves are listed as $\ell_1, \ell_2, \dots, \ell_m$ from left to right in T , where $1 \leq \ell_j \leq m$ for each j . Then, there exists j_0 such that ℓ_{j_0} and ℓ_{j_0+1} are siblings. Let p_0 be their parent. Then, $T - \{\ell_{j_0}, \ell_{j_0+1}\}$ has $m - 1$ leaves including p_0 .

By Lemma 2, $T - \{\ell_{j_0}, \ell_{j_0+1}\}$ is displayed as a base in the first $2m - 4$ rows such that (i) ℓ_j ($1 \leq j < j_0$) is mapped to $t_{(m-2)j}$, (ii) p_0 is mapped to $t_{(m-2)j_0}$, and (iii) ℓ_j ($j_0 + 1 < j \leq m$) is mapped to $t_{(m-2)(j-1)}$. Note that all the leaves in $T - \{\ell_{j_0}, \ell_{j_0+1}\}$ are one-to-one assigned to the tree vertexes in R_{2m-4} .

The display of $T - \{\ell_{j_0}, \ell_{j_0+1}\}$ can be extended into a display of T only by (i) reassign ℓ_j to $t_{(m-1)j}$ for $j < j_0$, (ii) assign ℓ_{j_0} and ℓ_{j_0+1} to $t_{(m-1)j_0}$ and $t_{(m-1)(j_0+1)}$, (iii) reassign ℓ_j to $t_{(m-1)j}$ for $j_0 + 1 < j \leq m - 1$, and (iv) assign ℓ_m to t_{mm} . It can be verify that such a display of T does not have any dummy vertex.

Define $\pi = (\ell_1 \ell_2 \dots \ell_m)$. Clearly, π is a one-to-one mapping over X , which maps i to ℓ_i . By Lemma 2, there are vertex-disjoint paths that cover every vertex and connect $t_{(m-1)j}$ and $t_{(2m-1)\ell_j}$ ($1 \leq j \leq m - 1$) and t_{mm} to $t_{(2m-1)\ell_m}$ in U_{lower} . Combining the display of T and the m disjoint paths, we conclude that T is a tree base for U . \square

CONCLUDING REMARKS

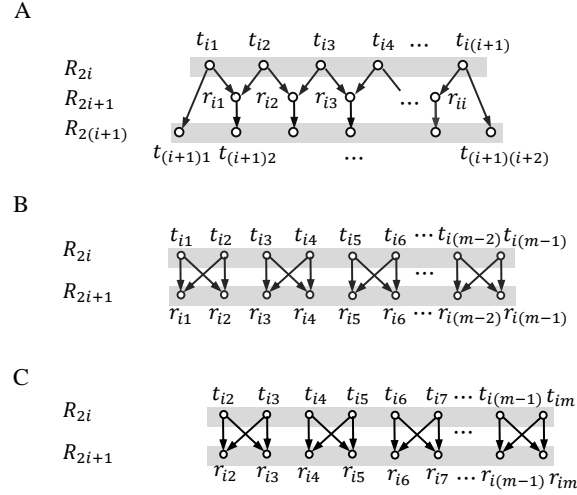


Figure 5: (A) The edges between vertexes in the rows $2i$, $2i + 1$ and $2(i + 1)$ in the upper part U_{top} for each i . (B) The edges between vertexes in the rows $2i$ and $2i + 1$ in the lower part U_{top} for $i = m - 1, m + 1, \dots, 2m - 2$. (C) The edges between the vertexes in the rows $2i$ and $2i + 1$ in the lower part for $i = m, m + 2, \dots, 2m - 3$. Here m is odd.

The universal tree-based network we have constructed has an important implication. A class of phylogenetic networks is said to be *complete* if every collection of phylogenetic trees on a set of species can be displayed in a phylogenetic network on the same species in the class. We use U_X to denote the universal tree-based network on X for a set X of species. Since every phylogenetic tree on X is displayed in U_X , the class of tree-based networks is complete.

In contrast, the class of reticulation visible networks is incomplete as well as its subclasses such as galled trees (Wang *et al.*, 2001) and galled networks. In fact, since a reticulation visible network over X has at most $4(n - 1)$ reticulation vertexes (Gambette *et al.*, 2015), more than $2^{4(n-1)}$ different trees on X cannot all be displayed in a reticulation visible phylogenetic tree simultaneously.

The completeness suggests that tree based networks are widespread in the entire space of phylogenetic networks. The simple linear time algorithm for testing whether a phylogenetic network is tree-based or not, given here, is definitely useful for further examination of the distribution of tree based networks.

Finally, tree-based networks are a natural model for horizontal gene transfer. They also compose a large complete class. Therefore, it is important to study how to reconstruct a tree-based network with as few reticulation vertexes as possible from a set of gene trees or from sequence data in future.

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APPENDIX A

Proof of Lemma 2.

Let $m \geq 3$. Recall that R_i denotes the set of vertexes in the row i in U . Let U_{2k-2} be the subnetwork consisting of vertexes in the top $2(k-1)$ rows in U_{upper} , $k = 2, 3, \dots, m-2$. The leaves in U_{2k-2} are all the tree vertexes $t_{(k-1)1}, t_{(k-1)2}, \dots, t_{(k-1)k}$ in R_{2k-2} . Note that $U_{2m-4} = U_{\text{upper}} - \{r_{(m-2)j} \mid 1 \leq j \leq m-2\}$.

For each k , a vertex in a subtree of U_{2k-2} is said to be a dummy leaf if it is not in the lowest level R_{2k-2} , but has out-degree 0. We prove that every phylogenetic tree with k leaves is a base of U_{2k-2} by induction on k .

When $k = 2$, N_2 is the unique binary tree with 2 leaves. Therefore, the statement is true.

Assume the statement is true for $k-1$. Let T be a phylogenetic tree with k leaves.

The depth of a vertex in a rooted tree is defined to be the number of edges in the path from the root to the vertex in the tree. The depth of the root is set to 0. Let ℓ' be the leaf with the largest depth in T . The sibling ℓ'' of ℓ' must be also a leaf of T . (If ℓ'' were not a leaf, its children would have a greater depth than ℓ' .) We use $p(\ell')$ to denote the parent of ℓ' and ℓ'' in T . Clearly, $T' = T - \{\ell', \ell''\}$ is a tree with $j-1$ leaves, one of which is $p(\ell')$.

By the induction hypothesis, T' is a base of $U_{2(k-1)-2} = U_{2k-4}$. Let $E' \subset \mathcal{E}(U_{2k-4})$ such that $U_{2k-4} - E'$ is a subdivision of T' in which there is no dummy leaf and all the leaves of T' correspond one-to-one the tree vertexes $t_{(k-2)j}$ ($1 \leq j \leq k-2$) in the row R_{2k-4} . Assume that $p(\ell')$ corresponds to $t_{(k-2)j_0}$ for some $1 \leq j_0 \leq k-2$.

Define $E'' = \{(t_{(k-2)j}, r_{(k-2)j}) \mid j < j_0\} \cup \{(t_{(k-2)j}, r_{(k-2)(j-1)}) \mid j > j_0\}$. Then, $N_k - E' - E''$ is a subdivision of T in which (i) there is no dummy leaf, (ii) the j th leaf corresponds to the j th vertex $t_{(k-1)j}$ in R_{2k-2} for $j < j_0$, (iii) ℓ' and ℓ'' correspond to $t_{(k-1)j_0}$ and $t_{(k-1)(j_0+1)}$, respectively, and (iv) the j th leaf corresponds to the j th vertex $t_{(k-1)(j+1)}$ in R_{2k-2} for $j \geq j_0 + 1$.

This concludes the proof of Lemma 2. \square

The structure of U_{lower}

When m is odd, U_{lower} consists of the last $2m+1$ rows in U : $R_{2m-2}, R_{2m-1}, \dots, R_{4m-2}$.

For $i = m-1, m+1, \dots, 2m-2$, R_{2i} comprises $m-1$ tree vertexes t_{ij} ($1 \leq j \leq m-1$). R_{2i+1} comprises $m-1$ reticulation vertexes r_{ij} ($1 \leq j \leq m-1$).

For $i = m, m+2, \dots, 2m-3$, R_{2i} comprises $m-1$ tree vertexes t_{ij} ($2 \leq j \leq m$); R_{2i+1} comprises $m-1$ reticulation vertexes $m-1$ r_{ij} ($2 \leq j \leq m$).

The last row R_{4m-2} comprises m leaves each labelled with ℓ_j ($1 \leq j \leq m$) from left to right. For sake of convenience, the j -th leaf is denoted by $t_{(2m-1)j}$.

The edges in U_{lower} include:

$$\begin{aligned}
(\text{Vertical edges}) \quad & (t_{ij}, r_{ij}), \ 1 \leq j \leq m-1, \ i = m-1+2k, \ 0 \leq k \leq (m-1)/2; \\
& (t_{ij}, r_{ij}), \ 2 \leq j \leq m, \ i = m+2k, \ 0 \leq k \leq (m-3)/2; \\
& (r_{ij}, t_{(i+1)j}), \ 2 \leq j \leq m-1, \ m-1 \leq i \leq 2m-3; \\
& (r_{i1}, t_{(i+2)1}), \ i = (m-1)+2k, \ 0 \leq k \leq (m-3)/2; \\
& (r_{im}, t_{(i+2)m}), \ i = m+2k, \ 0 \leq k \leq (m-3)/2; \\
& (r_{(2m-2)1}, t_{(2m-1)1}); \\
(\text{Diagonal edges}) \quad & (t_{ij}, r_{i(j+1)}), \ (t_{i(j+1)}, r_{ij}), \\
& \quad j = 1, 3, \dots, m-2, \ i = m-1+2k, \ 0 \leq k \leq (m-1)/2; \\
& (t_{ij}, r_{i(j+1)}), \ (t_{i(j+1)}, r_{ij}), \\
& \quad j = 2, 4, \dots, m-1, \ i = m+2k, \ 0 \leq k \leq (m-3)/2;
\end{aligned}$$

Finally, there are m edges connecting m vertexes at the bottom in U_{upper} and the corresponding vertexes in U_{lower} :

$$\begin{aligned}
& (t_{(m-2)1}, t_{(m-1)1}), \ (t_{(m-2)(m-1)}, t_{mm}), \\
& (r_{(m-2)j}, t_{(m-1)(j+1)}), \ j = 1, 2, \dots, m-2.
\end{aligned}$$

When m is even, N_{lower} also has $2m+1$ levels, each has m or $m-2$ vertexes, as shown in Figure 6.

For $i = m-1, m+1, \dots, 2m-3$, R_{2i} comprises m tree vertexes t_{ij} ($1 \leq j \leq m$), and R_{2i+1} comprises m reticulation vertexes r_{ij} ($1 \leq j \leq m$).

For $i = m, m+2, \dots, 2m-2$, R_{2i} comprises $m-2$ tree vertexes t_{ij} ($2 \leq j \leq m-1$), and R_{2i+1} comprises $m-2$ reticulation vertexes r_{ij} ($2 \leq j \leq m-1$).

The last row R_{4m-2} consists of m leaves with labels ℓ_j from left to right, denoted by $t_{(2m-1)j}$ ($1 \leq j \leq m$).

U_{lower} contains the following edges:

$$\begin{aligned}
(\text{Vertical edges}) \quad & (t_{ij}, r_{ij}), \ (r_{ij}, t_{(i+1)j}), \\
& \quad 2 \leq j \leq m-1, \ m-1 \leq i \leq 2(m-1); \\
& (r_{i1}, t_{(i+2)1}), \ (r_{im}, t_{(i+2)m}), \\
& \quad i = m-1+2k, \ 0 \leq k \leq (m-2)/2; \\
(\text{Diagonal edges}) \quad & (t_{ij}, r_{i(j+1)}), \ (t_{i(j+1)}, r_{ij}), \\
& \quad j = 1, 3, \dots, m-1, \\
& \quad i = m-1+2k, \ 0 \leq k \leq (m-2)/2; \\
& (t_{ij}, r_{i(j+1)}), \ (t_{i(j+1)}, r_{ij}), \\
& \quad j = 2, 4, \dots, m-2, \\
& \quad i = m+2k, \ 0 \leq k \leq (m-2)/2.
\end{aligned}$$

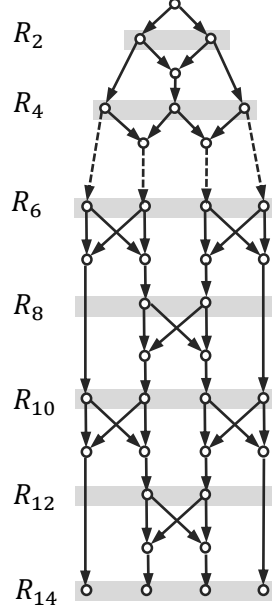


Figure 6: A universal network U with four leaves. Here, the square dot arrows represent the edges between the upper and lower parts.

Finally, there are m edges connecting the m vertexes in U_{upper} and the corresponding vertexes in U_{lower} :

$$\begin{aligned} & (t_{(m-2)1}, t_{(m-1)1}), (t_{(m-2)(m-1)}, t_{(m-1)m}), \\ & (r_{(m-2)j}, t_{(m-1)(j+1)}), \quad j = 1, 2, \dots, m-2. \end{aligned}$$

Proof of Lemma 3.

We first consider the case m is even. We define $m+1$ vectors S_i on $\{1, 2, \dots, m\}$ ($0 \leq i \leq m$). We use $S_i[j]$ to denote its j -th component for $1 \leq j \leq m$.

Initially, $S_0 = (\pi(1), \pi(2), \dots, \pi(m))$. After S_i is computed, we compute S_{i+1} as follows.

When i is even, S_{i+1} is defined by:

$$S_{i+1}[j] = \begin{cases} S_i[j] & \text{if } S_i[j] \leq S_i[j+1]; \\ S_i[j+1] & \text{if } S_i[j] > S_i[j+1] \end{cases}$$

and

$$S_{i+1}[j+1] = \begin{cases} S_i[j+1] & \text{if } S_i[j] \leq S_i[j+1]; \\ S_i[j] & \text{if } S_i[j] > S_i[j+1] \end{cases}$$

for $j = 1, 3, \dots, m-1$.

When i is odd, S_{i+1} is defined by:

$$\begin{aligned} S_{i+1}[1] &= S_i[1], \\ S_{i+1}[m] &= S_i[m], \end{aligned}$$

$$S_{i+1}[j] = \begin{cases} S_i[j] & \text{if } S_i[j] \leq S_i[j+1]; \\ S_i[j+1] & \text{if } S_i[j] > S_i[j+1] \end{cases}$$

and

$$S_{i+1}[j+1] = \begin{cases} S_i[j+1] & \text{if } S_i[j] \leq S_i[j+1]; \\ S_i[j] & \text{if } S_i[j] > S_i[j+1] \end{cases}$$

for $j = 2, 4, \dots, m-2$.

Since we emulate the odd-even transposition sorting on an array with m elements (Leighton, 1992, page 129), $S_m = (\pi(1), \pi(2), \dots, \pi(m))$. Using S_i 's, we obtain m vertex-disjoint paths connecting $t_{(m-1)i}$ and $t_{(2m-1)\pi(i)}$ as follows:

For $k = m-1, m+1, \dots, 2m-3$, and $j = 1, 3, \dots, m-1$, delete the vertical edges (t_{kj}, r_{kj}) and $(t_{k(j+1)}, r_{k(j+1)})$ if $S_{k-m+2}[j] = S_{k-m+1}[j+1]$ and $S_{k-m+2}[j+1] = S_{k-m+1}[j]$; and delete the diagonal edges $(t_{kj}, r_{k(j+1)})$ and $(t_{k(j+1)}, r_{kj})$ if $S_{k-m+2}[j] = S_{k-m+1}[j]$ and $S_{k-m+2}[j+1] = S_{k-m+1}[j+1]$.

For $k = m, m+2, \dots, 2m-2$, and $j = 2, 4, \dots, m-2$, delete the vertical edges (t_{kj}, r_{kj}) and $(t_{k(j+1)}, r_{k(j+1)})$ if $S_{k-m+2}[j] = S_{k-m+1}[j+1]$ and $S_{k-m+2}[j+1] = S_{k-m+1}[j]$, and delete the diagonal edges $(t_{kj}, r_{k(j+1)})$ and $(t_{k(j+1)}, r_{kj})$ if $S_{k-m+2}[j] = S_{k-m+1}[j]$ and $S_{k-m+2}[j+1] = S_{k-m+1}[j+1]$.

Since $S_m = (\pi(1), \pi(2), \dots, \pi(m))$, the resulting m vertex-disjoint paths connect $t_{(m-1)j}$ to $t_{(2m-1)\pi(i)}$ and pass through every vertex in U_{lower} .

For the case m is odd, we can prove the statement similarly. \square